Breaking the ties that bind: New hope for biomass fuels

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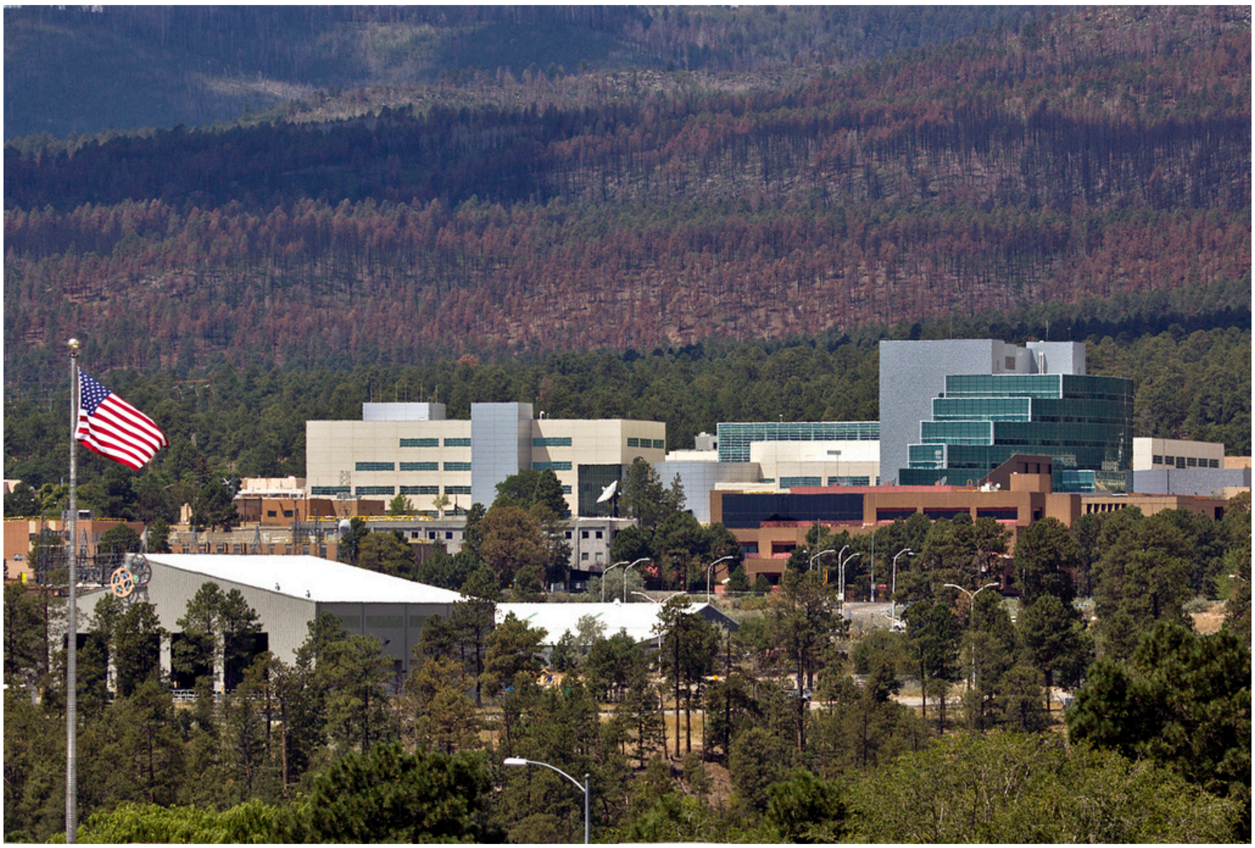

Los Alamos researchers crack code for binding lignocellulosic biomass

LOS ALAMOS, New Mexico, April 22, 2009—Los Alamos National Laboratory researchers have discovered a potential chink in the armor of fibers that make the cell walls of certain inedible plant materials so tough. The insight ultimately could lead to a cost-effective and energy-efficient strategy for turning biomass into alternative fuels.

In separate papers published today in *Biophysical Journal* and recently in an issue of Biomacromolecules, Los Alamos researchers identify potential weaknesses among sheets of cellulose molecules comprising lignocellulosic biomass, the inedible fibrous material derived from plant cell walls. The material is a potentially abundant source of sugar that can be used to brew batches of methanol or butanol, which show potential as biofuels.

Cellulose is biosynthesized in plant cells when molecules of glucose—a simple sugar—join into long chains through a process called polymerization. The plant then assembles these chains of cellulose into sheets. The sheets are held together by hydrogen bonds—an electrostatic attraction of a positive portion of a molecule to a negative portion of the same or neighboring molecule. Finally, the sheets stack atop one another, sticking to themselves by other types of attractions that are weaker than hydrogen bonds. The plant then spins these sheets into high-tensile-strength fibers of material.

Not only are the fibers incredibly strong, but they are incredibly resistant to the action of enzymes called cellulases that can crack the fibers back into their simple-sugar components. The ability to economically and easily break cellulose into sugars is desirable because the sugars can be used to create fuel alternatives. However, due to the tenacity of cellulose fibers, the United States currently lacks an energy-efficient and cost-effective method for turning inedible biomass such as switch grass or corn husks into a sweet source of biofuels.

Working with researchers from the U.S. Department of Agriculture and the Centre de Recherches sur les Macromolécules Végétales in France, Los Alamos researcher Paul Langan used neutrons to probe the crystalline structure of highly crystalline cellulose, much like an X-ray is used to probe the hidden structures of the body. Langan and his colleagues found that although cellulose generally has a well-ordered network of hydrogen bonds holding it together, the material also displays significant amounts of disorder, creating a different type of hydrogen bond network at certain surfaces. These differences make the molecule potentially vulnerable to an attack by cellulase enzymes.

Moreover, in this month's Biophysical Journal, Los Alamos researchers Tongye Shen and Gnana Gnanakaran describe a new lattice-based model of crystalline cellulose. The model predicts how hydrogen bonds in cellulose can shift to remain stable under a wide range of temperatures. This plasticity allows the material to swap different types of hydrogen bonds but also constrains the molecules so that they must form bonds in the weaker configuration described by Langan and his colleagues. Most important, Shen and Gnanakaran's model identifies hydrogen bonds that can be manipulated via temperature differences to potentially make the material more susceptible to attack by enzymes that can crack the fibers into sugars for biofuel production.

"We have been able to identify a chink in the armor of a very tough and worthy adversary—the cellulose fiber," said Gnanakaran, who leads the theoretical portion of a large, multidisciplinary biofuels project at Los Alamos.

"These results are some of the first to come from this team, and eventually could point us toward an economical and viable process for making biofuels from cellulosic biomass," adds Langan, director of the biofuels project.

Funding for the project comes from Laboratory-Directed Research and Development (LDRD), which is the premier source of internally directed research-and-development funding at Los Alamos National Laboratory. The LDRD program invests in high-risk, potentially high-payoff projects at the discretion of the Laboratory Director. Strategic investments of the LDRD program help position Los Alamos to anticipate and prepare for emerging national security challenges.